

Is the Adiabatic Approximation Inconsistent?

Solomon Duki¹, H. Mathur¹, and Onuttom Narayan²

¹*Department of Physics, Case Western Reserve University,
10900 Euclid Avenue, Cleveland OH 44106-7079*

²*Department of Physics, University of California, Santa Cruz, CA 95064*

In recent Letters Marzlin and Sanders [7] and Tong *et al.* [8] study an adiabatically varying Hamiltonian $h(t)$ that generates the time evolution $U(t)$ and its dual $H(t)$ that generates the evolution $U^\dagger(t)$. Marzlin and Sanders show that inconsistent results are obtained if an adiabatic approximation is used to calculate $H(t)$; Tong *et al.* show that the adiabatic approximation can be very inaccurate when applied to the exact dual Hamiltonian $H(t)$ even if it is an excellent approximation for $h(t)$. We show that these two observations are equivalent and are not inconsistent with the adiabatic theorem because in general, even if $h(t)$ satisfies the conditions of the adiabatic theorem, $H(t)$ will likely violate those conditions.

The adiabatic theorem is the basis of an approximation scheme that was discovered at the dawn of quantum mechanics [1] and that has been in widespread and continuous use ever since. Applications range from two-level systems (such as nuclei undergoing magnetic resonance or atoms interacting resonantly with a laser field) to quantum field theory (where a low-energy effective theory is derived by integrating out fast, high-energy degrees of freedom). Two decades ago, Berry uncovered the beautiful geometric structure underlying the adiabatic approximation [2], leading to a resurgence of interest in the subject and to new applications [3, 4]. More recently, it has been proposed that Berry phase effects lead to quantum phase transitions that lie outside the usual Landau-Ginzburg-Wilson paradigm [5]. The adiabatic theorem is also the basis of a newly proposed quantum computing scheme [6]. Considering the significance of the adiabatic approximation to quantum physics, the discovery of an inconsistency would be most disturbing. In a recent Letter Marzlin and Sanders [7] ask whether such an inconsistency might exist, at least for a class of Hamiltonians. That question has been further studied by Tong *et al.* [8] and subsequently commented on in Refs [9, 10]. The purpose of this Letter is to show that there is no inconsistency.

Refs [7] and [8] start with a time-dependent Hamiltonian $h(t)$ for which it is presumed that the adiabatic approximation is accurate. The evolution operator for $h(t)$ is denoted by $U(t)$, the solution to

$$i\frac{\partial}{\partial t}U(t) = h(t)U(t), \quad (1)$$

with $U(0) = \mathcal{I}$, where \mathcal{I} is the identity operator. Next, they consider the dual Hamiltonian $H(t)$ for which the evolution operator is $U^\dagger(t)$. Evidently

$$H(t) = -U^\dagger(t)i\frac{\partial}{\partial t}U(t) = -U^\dagger(t)h(t)U(t). \quad (2)$$

Tong *et al.* now formulate the putative inconsistency as follows: First they argue that $H(t)$ satisfies the conditions for the adiabatic theorem as well as does $h(t)$. Then they demonstrate that the adiabatic approximation can be very inaccurate for the dual Hamiltonian. These conflicting observations constitute the “inconsistency”. Marzlin and Sanders [7] originally formulated the inconsistency in a different form; below we will show the equivalence of the two formulations.

In this Letter we examine the dual Hamiltonian $H(t)$ and find it violates well known adiabaticity conditions; hence there is no inconsistency. The chief difficulty in determining whether $H(t)$ satisfies adiabatic conditions is that we do not have an explicit expression for $H(t)$ except in the special cases where the dynamics of $h(t)$ are simple enough to allow evaluation of $U(t)$. Nonetheless, we are able to give a general argument that $H(t)$ violates the conditions of the adiabatic theorem. As an illustration, we apply our general arguments to a solvable two-level model also studied by ref [8]. In this case it is possible to obtain the explicit form of $H(t)$; inspection of this form is sufficient to show immediately that $H(t)$ violates the conditions of the adiabatic theorem, consistent with our result.

It is helpful to first review the conditions under which the adiabatic approximation is accurate. Consider a two-level system with the Schrödinger equation

$$i\frac{\partial}{\partial t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \omega_0 & \Omega e^{-i\omega t} \\ \Omega e^{i\omega t} & -\omega_0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}. \quad (3)$$

We regard the off-diagonal terms as a perturbation and ask when the perturbation may be neglected. Evidently, the perturbation must be small in magnitude, but even if it is, it can have a big effect on resonance when $\omega \approx \omega_0$. This is more transparent if we go over to the interaction picture by writing $c_1 = a_1 \exp(-i\omega_0 t/2)$, $c_2 = a_2 \exp(i\omega_0 t/2)$. In the in-

interaction picture

$$i \frac{\partial}{\partial t} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & \Omega e^{-i(\omega - \omega_0)t} \\ \Omega e^{i(\omega - \omega_0)t} & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}. \quad (4)$$

Away from resonance the off-diagonal terms oscillate rapidly and average to zero. Near resonance, the perturbation varies slowly in the interaction picture and can have a big effect, producing Rabi oscillations. The precise condition to be off-resonance is $|\omega - \omega_0| \gg \Omega$. For this problem, the condition can be derived by transforming to another rotating frame via $a_1 = b_1 \exp[-i(\omega - \omega_0)t/2]$, $a_2 = b_2 \exp[i(\omega - \omega_0)t/2]$. In this frame, the Hamiltonian is time independent and equal to $(1/2)[(\omega - \omega_0)\sigma_z + \Omega\sigma_x]$. In summary, we need the perturbation to be off-resonance ($\Omega \ll |\omega - \omega_0|$) for it to be truly negligible.

Now let us consider the problem of a general time dependent hamiltonian $h(t)$. It is helpful to use a slightly different approach from the one above, which is useful for adiabatic perturbations. To this end, we introduce the instantaneous eigenstates $|n(t)\rangle$ that satisfy

$$h(t)|n(t)\rangle = \epsilon_n(t)|n(t)\rangle. \quad (5)$$

We choose the phases of $|n(t)\rangle$ to satisfy $\langle n(t)|\partial/\partial t|n(t)\rangle = 0$, a convention called the parallel transport gauge [11]. We expand the state of the system $|\psi\rangle$ in this time-dependent basis. Thus

$$|\psi(t)\rangle = \sum_n \phi_n(t) \exp[-i \int_0^t dt' \epsilon_n(t')] |n(t)\rangle. \quad (6)$$

In this moving frame the time-dependent Schrödinger equation has the form

$$i \frac{\partial}{\partial t} \phi_n(t) = \sum_{m \neq n} A_{nm}(t) \exp(i \int_0^t dt' [\epsilon_n(t') - \epsilon_m(t')]) \phi_m(t). \quad (7)$$

Here

$$A_{nm}(t) = -i \langle n | \frac{\partial}{\partial t} | m \rangle. \quad (8)$$

The adiabatic approximation amounts to neglect of the terms on the right hand side of eq (7). For this to be justified, by analogy to eq (4), we see that the neglected terms must be off-resonance. Roughly the condition to be off-resonance is that the neglected terms should *not* vary slowly; i.e. the terms should be small in magnitude compared to their predominant frequency. Note that this is somewhat different from the adiabatic condition $|A_{nm}| \ll |\epsilon_n - \epsilon_m|$ used by refs [7, 8]. More precisely, if the Hamiltonian varies predominantly at a frequency ω , and the typical spacing between instantaneous eigenvalues is Δ , our adiabatic condition states

$|A_{nm}| \ll (\Delta - \omega)$. Alternatively, if the Hamiltonian varies on a time scale T for which $1/\Delta T \ll 1$, and $A_{nm} \sim 1/T$, the correction to the adiabatic approximation is $\sim 1/\Delta T$ which is very small. This condition is more restrictive than necessary, but it agrees with the intuitive expectation that for the adiabatic approximation to apply, the Hamiltonian must “vary slowly”.

Sampling the literature we find that the graduate text by Schiff [12] gives a rather complete discussion of the adiabatic approximation, emphasizing that the neglected terms must be non-resonant. On the other hand, Landau and Lifshitz [13] give the more restrictive adiabatic condition $T \rightarrow \infty$. Moody, Shapere and Wilczek [14] compute non-perturbative corrections to adiabatic evolution using $1/\Delta T$ as the small parameter. Berry [15] also regards $1/\Delta T$ as the adiabatic parameter and suggests that the corrections vanish as $\exp(-\Delta T)$, also proposed by Hwang and Pechukas [16]. Thus it appears to be generally accepted that it is sufficient for the Hamiltonian to be slowly varying, but less restrictive conditions are also discussed.

For the dual Hamiltonian $H(t)$, denote the instantaneous eigenstates $|n(t); H\rangle$ and the eigenvalues $\epsilon_n^H(t)$. With the parallel transport gauge, in the adiabatic frame

$$|\psi(t)\rangle = \sum_n \phi_n^H(t) \exp[-i \int_0^t dt' \epsilon_n^H(t')] |n(t); H\rangle. \quad (9)$$

By analogy to eq (7) the Schrödinger equation obeyed by the amplitudes $\phi_n^H(t)$ is

$$i \frac{\partial}{\partial t} \phi_n^H(t) = \sum_{m \neq n} A_{nm}^H(t) \exp(i \int_0^t dt' [\epsilon_n^H(t') - \epsilon_m^H(t')]) \phi_m^H(t). \quad (10)$$

Although, as noted above, we do not have an explicit expression for $H(t)$, it is easy to relate the eigenstates of H to those of h . Evidently $U^\dagger(t)|n(t)\rangle$ is an eigenstate of $H(t)$ with eigenvalue $-\epsilon_n(t)$. Hence we write

$$\begin{aligned} |n(t); H\rangle &= U^\dagger(t)|n(t)\rangle \exp[-i \int_0^t dt' \epsilon_n(t')]; \\ \epsilon_n^H(t) &= -\epsilon_n(t). \end{aligned} \quad (11)$$

The phase of $|n(t); H\rangle$ has been chosen to ensure parallel transport, $\langle n; H | \partial_t | n; H \rangle = 0$. To verify this, it is helpful to recall that $iU\partial_t U^\dagger = -h$, which follows from the Schrödinger equation (1). Using eq (11) and this result, one can show that

$$A_{nm}^H(t) = A_{nm}(t) \exp(i \int_0^t dt' [\epsilon_m(t') - \epsilon_n(t')]). \quad (12)$$

Substituting eq (12) into eq (10) we obtain the final form of the Schrödinger equation in the adiabatic frame

for the dual Hamiltonian $H(t)$,

$$i \frac{\partial}{\partial t} \phi_n^H(t) = \sum_{m \neq n} A_{nm}(t) \phi_m^H(t). \quad (13)$$

Eq (13) is the main result of our general analysis.

Eq (13) shows that the terms that would be neglected in the adiabatic approximation $A_{nm}(t)$ vary slowly. The typical frequency of these terms is $1/T$, the same as their magnitude. Thus $H(t)$ does not fulfil the adiabatic condition, and using the adiabatic approximation for $H(t)$ leads to inaccurate results.

This concludes our general analysis of $H(t)$. We turn to a solvable example. Take the two-level Hamiltonian

$$h(t) = -\frac{1}{2}\omega_0 \begin{pmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{pmatrix} \quad (14)$$

Physically we can picture this as a spin $\frac{1}{2}$ particle in a magnetic field tilted at an angle θ to the z -axis and rotating at a frequency ω . Essentially this model was also studied in ref [8]. The instantaneous eigenvalues of this Hamiltonian are $\varepsilon_{\pm}(t) = \pm\omega_0/2$; the corresponding eigenspinors in the parallel transport gauge are [17]

$$\begin{aligned} |+(t)\rangle &= \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\omega t} \end{pmatrix} \exp[-i\frac{\omega t}{2}(1 - \cos \theta)], \\ |- (t)\rangle &= \begin{pmatrix} -\sin \frac{\theta}{2} e^{-i\omega t} \\ \cos \frac{\theta}{2} \end{pmatrix} \exp[i\frac{\omega t}{2}(1 - \cos \theta)] \end{aligned} \quad (15)$$

A straightforward computation reveals that

$$A_{+-}(t) = \langle + | \partial_t | - \rangle = \frac{\omega}{2} \sin \theta e^{-i\omega t \cos \theta}. \quad (16)$$

It follows from eq (7) that the adiabatic frame Schrödinger equation for $h(t)$ is

$$i \frac{\partial}{\partial t} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} = \begin{pmatrix} 0 & A_{+-} e^{i\omega_0 t} \\ A_{+-}^* e^{-i\omega_0 t} & 0 \end{pmatrix} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}. \quad (17)$$

Clearly for the off-diagonal term to be off-resonance, we need $|\omega \cos \theta - \omega_0| \gg \omega \sin \theta$. Evidently, this condition is satisfied if $\omega \ll \omega_0$, *i.e.*, $h(t)$ varies slowly.

It follows from eq (13) that the adiabatic frame Schrödinger equation for $H(t)$ is

$$i \frac{\partial}{\partial t} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} = \begin{pmatrix} 0 & A_{+-}(t) \\ A_{+-}^*(t) & 0 \end{pmatrix} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}. \quad (18)$$

Clearly, for the off-diagonal term to be off-resonance we need $|\omega \sin \theta| \ll |\omega \cos \theta|$, a condition met only when $\theta \ll 1$ (or $\pi - \theta \ll 1$).

In summary we find that for $h(t)$ to be adiabatic it is sufficient that $\omega \ll \omega_0$; but for $H(t)$ to be adiabatic we

also need $\theta \ll 1$. In this limit, $\theta \rightarrow 0$, the fidelity of the adiabatic solution to $H(t)$ (the overlap of the adiabatic and exact solutions) computed by [7, 8] approaches unity, consistent with our finding.

We note that in this solvable problem it is possible to compute U and explicitly obtain $H(t)$. This column is far too narrow to write the entire expression, but it includes terms that oscillate at a frequency

$$\nu = \sqrt{\omega_0^2 + \omega^2 + 2\omega_0\omega \cos \theta}. \quad (19)$$

In the limit $\omega \ll \omega_0$, needed for the Hamiltonian $h(t)$ to be adiabatically varying, $\nu \rightarrow \omega_0$. Thus, even without going to the adiabatic frame, a cursory inspection of $H(t)$ is sufficient to show it is not slowly varying and is unlikely to satisfy the adiabatic condition.

We briefly comment on cases where the adiabatic approximation applies to $h(t)$ and $H(t)$. This happens when there is a parameter other than T which can be tuned to make the magnitude of the off-diagonal term in eq (13) small compared to the predominant frequency $1/T$. However, for $h(t)$ the approximation becomes more accurate as $T \rightarrow \infty$ (with exponentially small corrections according to refs [14, 15, 16]), whereas for $H(t)$ the distance from resonance is essentially independent of T and is controlled by the additional parameter. This can be seen in the example above, where $T \rightarrow 2\pi/\omega$ and θ is the additional parameter.

We make a few observations in passing here about the discussion of the adiabatic conditions after Eq.(8). First, the effects of A_{nm} are implicitly integrated over a finite time window. This is appropriate, since in experiments $h(t)$ is typically varied only within a finite time window. However, it is the discontinuity in dh/dt that causes the $\sim 1/(\Delta T)$ correction to the adiabatic approximation for large T ; if all derivatives of $h(t)$ are continuous for all t , it is known [14, 15, 16] that the correction will be exponentially small in $T\Delta$. Second, Δ was effectively taken to be time independent. When both A_{nm} and Δ vary sinusoidally at frequency ω , higher order resonances result when $\omega = \Delta_0/k$ for integer k . This is essentially the same mechanism that causes resonances going beyond first order perturbation theory.

Finally we discuss the equivalence between the formulations of refs [7] and [8]. They assume that the adiabatic approximation is accurate for $h(t) : U(t) \approx U_{\text{adia}}(t)$ where

$$U_{\text{adia}}(t) = \sum_n |n(t)\rangle \langle n(0)| \exp \left[-i \int_0^t dt' \varepsilon_n(t') \right] \quad (20)$$

is the adiabatic approximation to the exact evolution $U(t)$. Marzlin *et al.* [7] then develop an approx-

imation to $U^\dagger(t)$ that we denote $V^\dagger(t)$. They approximate the dual Hamiltonian [defined by eq (2)] as $H_{\text{adia}}^{(1)}(t) = -U_{\text{adia}}^\dagger(t)h(t)U_{\text{adia}}(t)$. They compute the evolution $V^\dagger(t)$ corresponding to $H_{\text{adia}}^{(1)}(t)$, obtaining

$$V^\dagger(t) = \sum_n |n(0)\rangle\langle n(0)| \exp \left[i \int_0^t dt' \varepsilon_n(t') \right]. \quad (21)$$

In contrast, Tong *et al.* compute a different approximation to $U^\dagger(t)$ that we denote $W^\dagger(t)$. They work with the exact dual Hamiltonian $H(t)$, but work out its evolution using the adiabatic approximation. Analogy to eq (20) and use of eq (11) leads to the result

$$W^\dagger(t) = \sum_n U^\dagger(t) |n(t)\rangle\langle n(0)|. \quad (22)$$

The operators V^\dagger and W^\dagger are different in appearance and in the approximations that lead to them, but we will show they are equivalent to the extent that the adiabatic approximation $U \approx U_{\text{adia}}$ is valid.

With this notation established we now turn to the inconsistencies. Marzlin and Sanders [7] consider the identity $UU^\dagger = \mathcal{I}$ and replace $U \rightarrow U_{\text{adia}}$ and $U^\dagger \rightarrow V^\dagger$ with the disastrous result that $UU^\dagger \rightarrow \sum_n |n(t)\rangle\langle n(0)| \neq \mathcal{I}$. Tong *et al.* derive the same inconsistency by replacing U^\dagger with W^\dagger : $UU^\dagger \rightarrow UW^\dagger$ and using Eq.(22). The equivalence of the two approaches can be seen by starting with the trivial identity $U^\dagger = U^\dagger UU^\dagger$. If on the right hand side we replace $U^\dagger UU^\dagger \rightarrow U^\dagger U_{\text{adia}} V^\dagger$ we obtain W^\dagger by use of eqs (20), (21) and (22). In other words, the approximation of Marzlin and Sanders with the adiabatic approximation is equivalent to the approximation of Tong *et al.*

The resolution of the inconsistencies of Refs.[7, 8] is that $V^\dagger \approx U^\dagger$ and $W^\dagger \approx U^\dagger$ are not good approximations; the adiabatic approximation $U_{\text{adia}} \approx U$ is not at fault. In this Letter we have explained the failure of the approximation $W^\dagger \approx U^\dagger$. This may also be considered a resolution of the Marzlin and Sanders form of the inconsistency, due to the equivalence shown above. An alternative resolution was provided in ref [7] who used the adiabatic approximation to calculate a second approximation to the dual Hamiltonian $H_{\text{adia}}^{(2)}(t) = -iU_{\text{adia}}^\dagger \partial_t U_{\text{adia}}$. By construction, the evolution operator corresponding to $H_{\text{adia}}^{(2)}(t)$ is $U_{\text{adia}}^\dagger(t)$ which is indeed a good approximation to U^\dagger . Since the trustworthy adiabatic approximation has been used to compute both $H_{\text{adia}}^{(1)}(t)$ and $H_{\text{adia}}^{(2)}(t)$ we may presume that $H_{\text{adia}}^{(1)}(t) \approx H_{\text{adia}}^{(2)}(t) \approx H(t)$. This does not mean that the three Hamiltonians will generate essentially the same evolution since small errors can grow upon time exponentiation. Indeed ref [7] finds that $H_{\text{adia}}^{(1)}$

and $H_{\text{adia}}^{(2)}$ differ by a small resonant perturbation leading to the inference that V^\dagger may be very different from U_{adia}^\dagger . Since $U_{\text{adia}}^\dagger \approx U^\dagger$ this may be considered to explain the failure of the approximation $V^\dagger \approx U^\dagger$.

To summarise, we have studied the dual pair of Hamiltonians $h(t)$ and $H(t)$ that generate time evolution $U(t)$ and $U^\dagger(t)$ respectively. Marzlin and Sanders [7] showed that if an adiabatic approximation is used to compute $H(t)$ an inconsistency results. Tong *et al.* [8] showed that the same inconsistency results if the adiabatic approximation is applied to the exact dual Hamiltonian $H(t)$. We show that these observations are essentially equivalent. Our main finding is that even if $h(t)$ satisfies the conditions of the adiabatic theorem, $H(t)$ will not (except in the trivial case when the total change in $h(t)$ is small) because the terms neglected in the adiabatic approximation are resonant for $H(t)$. Thus the breakdown of the adiabatic approximation for H is not inconsistent with the adiabatic theorem.

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stantaneous eigenstates, eq (15), change according to $|\pm\rangle \rightarrow |\pm\rangle \exp(\mp i\gamma)$. Here $\gamma = \pi(1 - \cos\theta)$ is one half the solid angle traced by the magnetic field, the well-known Berry phase for this problem [2].